Incorporating Cobalt Carbonyl Moieties onto Ethynylthiophene-Based Dithienylcyclopentene Switches. 1. Photochemistry

Harvey, Emma C.; Areephong, Jetsuda; Cafolla, Attilio A.; Long, Conor; Browne, Wesley R.; Pryce, Mary T.; Feringa, Bernard

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Data for Quantum Chemical Calculations

Optimized Coordinates

Compound 1Ho

51 55

SMALL

NO_CHARGES

@<TRIPOS>ATOM

1 C1 -8.2089 -0.5094 -0.8173 C

2 C2 -7.2998 -1.1563 -0.0035 C

3 C3 -7.8631 -2.3472 0.5849 C

4 C4 -9.1544 -2.5654 0.2095 C

5 S5 -9.7279 -1.3307 -0.8710 S

6 H6 -8.0538 0.4009 -1.3790 H

7 H7 -7.3073 -2.9932 1.2544 H

8 H8 -9.8076 -3.3766 0.5007 H

9 C9 -5.9745 -0.7099 0.2293 C

10 C10 -4.8344 -0.3352 0.4365 C

11 C11 -3.5166 0.0867 0.6833 C

12 C12 -2.8582 1.1930 0.1957 C

13 S13 -2.4464 -0.8283 1.7392 S

14 C14 -1.4999 1.3152 0.6352 C

15 H15 -3.3347 1.8955 -0.4788 H

16 C16 -1.1340 0.2948 1.4964 C

17 C17 0.1654 0.0809 2.2131 C

18 H18 0.7000 1.0300 2.3084 H

19 H19 0.0063 -0.3280 3.2168 H

20	H20	0.8228	-0.6097	1.6703	H
21	C21	-0.6492	2.4571	0.2473	C
22	C22	-1.1538	3.8797	0.4525	C
23	C23	0.6229	2.4569	-0.2189	C
24	C24	-0.1126	4.7513	-0.2809	C
25	H25	-1.1954	4.1055	1.5292	H
26	H26	-2.1731	4.0271	0.0747	H
27	C27	1.1601	3.8789	-0.3314	C
28	H28	-0.4562	4.9484	-1.3032	H
29	H29	1.8332	4.1011	0.5117	H
30	H30	1.7476	4.0325	-1.2440	H
31	H31	0.0499	5.7202	0.2015	H
32	C32	1.4828	1.3166	-0.5848	C
33	C33	1.1238	0.2666	-1.4130	C
34	C34	3.5211	0.1242	-0.6290	C
35	C35	2.8494	1.2318	-0.1627	C
36	H36	3.3235	1.9636	0.4817	H
37	S37	2.4531	-0.8395	-1.6425	S
38	C38	-0.1779	0.0159	-2.1132	C
39	H39	-0.8279	-0.6584	-1.5420	H
40	H40	-0.7190	0.9578	-2.2402	H
41	H41	-0.0210	-0.4287	-3.1020	H
42	C42	4.8499	-0.2669	-0.3901	C
43	C43	5.9972	-0.6277	-0.1983	C
44	C44	7.3378	-1.0194	0.0450	C
45	C45	8.2582	-0.2756	0.8703	C
46	C46	9.4882	-0.8559	0.9503	C

47 H47 7.9881 0.6476 1.3696 H

48 H48 10.3560 -0.5117 1.4964 H

49 C49 7.9233 -2.1564 -0.4763 C

50 S50 9.5678 -2.3252 0.0255 S

51 H51 7.4658 -2.8910 -1.1238 H

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Complex 3Ho

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SMALL

NO_CHARGES

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2 C2 -5.7061 2.3789 -0.4250 C

3 C3 -4.5514 3.2233 -0.2415 C

4 C4 -4.7946 4.5322 -0.5349 C

5 S5 -6.4356 4.7804 -1.0477 S

6 H6 -7.7895 2.7297 -1.0658 H

7 H7 -3.5905 2.8529 0.0960 H

8 H8 -4.1084 5.3668 -0.4872 H

9 C9 -5.7219 0.9486 -0.1609 C

10 C10 -4.8779 -0.1197 -0.1201 C

11	C11	-3.5326	-0.5059	-0.4539	C
12	C12	-2.8381	-1.6227	-0.0550	C
13	S13	-2.5287	0.4551	-1.5370	S
14	C14	-1.5067	-1.7206	-0.5746	C
15	H15	-3.2706	-2.3591	0.6141	H
16	C16	-1.1999	-0.6682	-1.4201	C
17	C17	0.0505	-0.4215	-2.2099	C
18	H18	0.5816	-1.3636	-2.3717	H
19	H19	-0.1738	0.0205	-3.1865	H
20	H20	0.7376	0.2551	-1.6868	H
21	C21	-0.6260	-2.8667	-0.2769	C
22	C22	-1.1227	-4.2873	-0.5111	C
23	C23	0.6682	-2.8654	0.1225	C
24	C24	-0.0335	-5.1705	0.1339	C
25	H25	-1.2161	-4.4718	-1.5923	H
26	H26	-2.1192	-4.4643	-0.0880	H
27	C27	1.2294	-4.2820	0.1537	C
28	H28	-0.3218	-5.4121	1.1635	H
29	H29	1.8618	-4.4619	-0.7297	H
30	H30	1.8639	-4.4615	1.0294	H
31	H31	0.1168	-6.1169	-0.3942	H
32	C32	1.5281	-1.7238	0.4836	C
33	C33	1.2024	-0.7176	1.3761	C
34	C34	3.5454	-0.4870	0.4408	C
35	C35	2.8643	-1.5893	-0.0166	C
36	H36	3.3104	-2.2922	-0.7120	H
37	S37	2.5225	0.4084	1.5618	S

38	C38	-0.0543	-0.5246	2.1702 C
39	H39	-0.7531	0.1589	1.6720 H
40	H40	-0.5673	-1.4828	2.2921 H
41	H41	0.1591	-0.1178	3.1644 H
42	C42	4.8927	-0.0809	0.1369 C
43	C43	5.7381	0.9851	0.1631 C
44	C44	5.7669	2.4165	0.4123 C
45	C45	6.9745	3.2005	0.4337 C
46	C46	6.7527	4.5236	0.6713 C
47	H47	7.9594	2.7751	0.2773 H
48	H48	7.4782	5.3226	0.7419 H
49	C49	4.6530	3.1986	0.6376 C
50	S50	5.0598	4.8615	0.8736 S
51	H51	3.6198	2.8826	0.6695 H
52	Co52	6.6547	-0.5698	0.8774 Co
53	C53	6.3265	-0.2693	2.5940 C
54	C54	8.4077	-0.1486	0.8002 C
55	C55	6.6062	-2.3756	0.8481 C
56	O56	6.1183	-0.0640	3.7046 O
57	O57	6.5398	-3.5221	0.8256 O
58	O58	9.5202	0.1359	0.7448 O
59	Co59	6.0238	-0.1062	-1.4410 Co
60	C60	5.8901	-1.7971	-2.0544 C
61	C61	7.6173	0.4740	-2.0562 C
62	C62	4.9207	0.7442	-2.5388 C
63	O63	4.1899	1.2932	-3.2348 O
64	O64	5.7835	-2.8779	-2.4317 O

65 O65 8.6313 0.8612 -2.4327 O

66 Co66 -6.6529 -0.6059 -0.8315 Co

67 Co67 -5.9796 -0.1193 1.4736 Co

68 C68 -8.3960 -0.1441 -0.7522 C

69 C69 -6.6455 -2.4095 -0.7549 C

70 C70 -6.3273 -0.3634 -2.5586 C

71 C71 -7.5623 0.4881 2.0966 C

72 C72 -4.8561 0.7373 2.5423 C

73 C73 -5.8396 -1.8010 2.1125 C

74 O74 -4.1084 1.2870 3.2203 O

75 O75 -8.5667 0.8960 2.4754 O

76 O76 -5.7268 -2.8766 2.5028 O

77 O77 -6.1211 -0.1951 -3.6757 O

78 O78 -9.4999 0.1738 -0.7090 O

79 O79 -6.6085 -3.5563 -0.6994 O

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Complex 4Fo

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SMALL

NO_CHARGES

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1 C1 10.4302 -4.2090 0.1691 C

2 C2 9.5594 -3.2304 -0.2559 C

3 C3 8.4634 -3.7901 -1.0086 C

4 C4 8.5332 -5.1467 -1.1266 C

5 S5 9.9323 -5.7889 -0.3224 S

6 H6 11.3386 -4.0766 0.7407 H

7 H7 7.6714 -3.1893 -1.4414 H

8 H8 7.8467 -5.8101 -1.6351 H

9 C9 9.7271 -1.8075 -0.0048 C

10 C10 8.9880 -0.6739 0.1297 C

11 C11 7.5987 -0.2539 0.2843 C

12 C12 7.2033 1.0761 0.0547 C

13 C13 6.6113 -1.1718 0.6911 C

14 C14 5.8825 1.4717 0.2141 C

15 H15 7.9487 1.8080 -0.2420 H

16 C16 5.2878 -0.7771 0.8462 C

17 H17 6.8873 -2.2046 0.8811 H

18 C18 4.8915 0.5509 0.6058 C

19 H19 5.6147 2.5115 0.0533 H

20 H20 4.5466 -1.5165 1.1379 H

21 C21 3.4971 0.9796 0.7452 C

22	C22	2.8590	2.0242	0.1277	C
23	S23	2.3756	0.1495	1.8113	S
24	C24	1.4716	2.1543	0.4724	C
25	H25	3.3443	2.6767	-0.5879	H
26	C26	1.0592	1.2078	1.3941	C
27	C27	-0.2782	1.0349	2.0487	C
28	H28	-0.9218	0.3486	1.4846	H
29	H29	-0.1761	0.6409	3.0648	H
30	H30	-0.7986	1.9953	2.1077	H
31	C31	0.6366	3.2349	-0.0643	C
32	C32	-0.6314	3.2175	-0.5504	C
33	C33	1.2198	4.6282	-0.1433	C
34	C34	-1.0950	4.6144	-0.9032	C
35	C35	0.0004	5.5593	-0.3480	C
36	C36	-1.5032	2.0754	-0.8637	C
37	C37	-2.8785	2.0015	-0.4607	C
38	C38	-3.5295	0.8714	-0.8860	C
39	H39	-3.3478	2.7578	0.1553	H
40	C40	-1.1140	0.9942	-1.6351	C
41	S41	-2.4365	-0.1169	-1.8403	S
42	C42	0.2065	0.7189	-2.2898	C
43	H43	0.7263	1.6570	-2.5051	H
44	H44	0.8629	0.1199	-1.6462	H
45	H45	0.0777	0.1783	-3.2330	H
46	C46	-4.9184	0.4704	-0.6456	C
47	C47	-5.8996	1.4355	-0.3483	C
48	C48	-5.3202	-0.8770	-0.6970	C

49	C49	-7.2166	1.0678	-0.1064	C
50	H50	-5.6292	2.4867	-0.3280	H
51	C51	-6.6411	-1.2428	-0.4700	C
52	H52	-4.5858	-1.6518	-0.9005	H
53	C53	-7.6214	-0.2771	-0.1698	C
54	H54	-7.9508	1.8335	0.1251	H
55	H55	-6.9184	-2.2921	-0.5035	H
56	C56	-9.0018	-0.6760	0.0892	C
57	C57	-9.8703	-1.6878	-0.1746	C
58	C58	-10.0124	-2.8714	-1.0069	C
59	C59	-11.0370	-3.8662	-0.8291	C
60	C60	-10.9796	-4.8680	-1.7513	C
61	H61	-11.7761	-3.8202	-0.0372	H
62	H62	-11.6204	-5.7348	-1.8398	H
63	C63	-9.2033	-3.1665	-2.0853	C
64	H64	-8.3710	-2.5888	-2.4624	H
65	S65	-9.6772	-4.6285	-2.8761	S
66	Co66	-10.7807	0.0530	-0.1498	Co
67	Co67	-9.9306	-1.2768	1.7198	Co
68	Co68	10.5406	-0.6794	1.3382	Co
69	Co69	10.4565	-0.3290	-1.0841	Co
70	C70	10.6109	1.4681	-1.1421	C
71	C71	9.5872	-0.6346	-2.5964	C
72	C72	12.0986	-0.9452	-1.5186	C
73	C73	9.7661	-1.3916	2.7655	C
74	C74	10.6706	1.0432	1.8651	C
75	C75	12.2137	-1.3343	1.4966	C

76 C76 -9.5901 0.0580 2.8884 C

77 C77 -11.4760 -2.0114 2.2888 C

78 C78 -8.7638 -2.4929 2.2670 C

79 C79 -10.7194 1.6997 0.5879 C

80 C80 -12.5239 -0.4087 -0.0642 C

81 C81 -10.6399 0.4488 -1.8722 C

82 O82 -10.6709 2.7494 1.0533 O

83 O83 -13.6251 -0.7306 -0.0134 O

84 O84 -10.5296 0.6967 -2.9881 O

85 O85 -12.4621 -2.4925 2.6315 O

86 O86 -9.3551 0.9168 3.6137 O

87 O87 -8.0047 -3.2874 2.6026 O

88 O88 10.7345 2.1431 2.1887 O

89 O89 13.2702 -1.7765 1.5930 O

90 O90 9.2574 -1.8667 3.6792 O

91 O91 13.1329 -1.3673 -1.7838 O

92 O92 10.6978 2.6138 -1.1750 O

93 O93 9.0048 -0.8336 -3.5668 O

94 F94 -2.3107 4.9186 -0.3614 F

95 F95 -1.2106 4.7736 -2.2514 F

96 F96 0.2640 6.5884 -1.1765 F

97 F97 2.0673 4.7413 -1.2181 F

98 F98 1.9294 4.9750 0.9584 F

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